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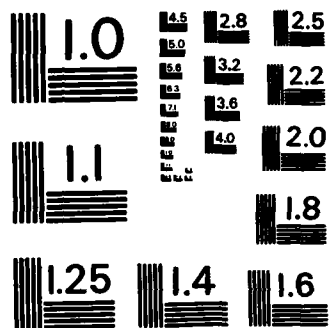
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WAVE REFLECTION AND QUASIRESONANCE

R. E. Meyer

Mathematics Research Center
University of Wisconsin-Madison
610 Walnut Street
Madison, Wisconsin 53706

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ABSTRACT

Wave reflection by smooth media and resonance of systems with radiation damping are instructive examples of a failure of the standard approach to asymptotics. They are also good examples of a type of exponential asymptotics needed for the sciences. Successful modifications of conventional, singular-perturbation theory have been found for them and show some of the principles promising wider usefulness. They have led to recent developments in WKB-connection theory, which are also reported briefly.

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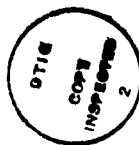
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SIGNIFICANCE AND EXPLANATION

Asymptotics plays a big role in science and technology because it is a form of mathematical analysis designed to produce highly illuminating results. The last decade has brought a rapidly increasing number of experiences -- in studies of chemical reactions mechanisms, population genetics, wave scattering and other matters of quite practical concern -- where subtle issues not accessible to established asymptotic methods turned out to be decisive. A few problems of this kind have been solved, but in a way accessible only to a small circle of specialists.

This article for a book uses two examples to explain to a wider, mathematically trained audience the typical issues encountered, the main ideas which have led to their resolution and the changes in the general approach to asymptotics which they portend.

One example concerns the common process of wave transmission and reflection in a stratified medium where, as the wavelength decreases, the whole issue begins to slip unresolved through the net of the established mathematical theory. The other, concerns unexpected resonance effects discovered in quantum chemistry, where understanding and prediction depend on making the old and the new asymptotics play equal and complementary roles.



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WAVE REFLECTION AND QUASIRESONANCE

R. E. Meyer

I. Wave Reflection?

We are creatures of habit and when a mathematical theory has enjoyed an initial success, it tends to develop further under its own steam, without much inquiry whether it really addresses the questions most seriously at issue. It may be of interest to look here at two examples from mathematical physics in which it has become apparent recently that asymptotic analysis has narrowly missed the true questions for a long time.

The first example is embarrassingly simple. When waves travel through a medium, the main practical questions concern transmission and reflection. More often than not, in fact, nothing else is observable. The main, classical transmission and reflection effects arise from boundaries, interfaces, cracks, etc., where a discontinuous change in material properties provides a reasonable model. Once such effects are understood, attention wanders to the modulation of the waves during travel through the medium, which is not normally a uniform one, but has properties varying continuously from place to place. It is hard to suppress a feeling that those variations are also a plausible cause of partial wave reflection and of correspondingly incomplete transmission, but little information on it can be found in textbooks.

To understand why, it will help to focus attention on the simplest circumstances in which the salient points stand out clearly. Boundaries and interfaces will be ignored, as will be processes by which one wave type, e.g. of compression, gradually generates another, e.g. of shear. The waves will be assumed linear and Fourier-analyzed into individual modes of frequency ω . The material will be assumed 'plane-layered' so that the phase velocity is a continuous function $c(x)$ of only one Cartesian coordinate x . Plane-wave propagation in the x -direction is then described by as simple a differential equation as

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$$d^2v/dx^2 + [n(x)/\epsilon]^2 v(x) = 0 \quad (1)$$

where

$$n(x) = c_0/c(x), \quad \epsilon = c_0/\omega$$

in terms of a reference value c_0 of c . Shortwave theory covers, first of all, the case of small wavelength scale ϵ , but it also tends to concern most of what we normally think of as waves: if $\epsilon > 1/3$, say, the solutions will not be recognizably waves because their shape will change too rapidly from place to place for an impression even of the notion of wave length. The function $n(x)$ describes the medium and has various names, of which the optical one, "index of refraction", will be used here. Its definition makes it natural to expect

$$n(x) > 0 \quad (2)$$

and this will be assumed. For waves obliquely incident on the layered medium, the following applies as long as the obliqueness is not too strong for (2); the formation of caustics is here excluded in the interest of simplicity (but it will be central to the second example).

A classical definition of transmission and reflection also requires reference to clear-cut, unmodulated wave states that can be compared unambiguously. This demands an assumption that the medium approaches homogeneity far from the region of notable modulation,

$$\begin{aligned} n(x) &\rightarrow n_+ > 0 \quad \text{as } x \rightarrow +\infty \\ &\rightarrow n_- > 0 \quad \text{as } x \rightarrow -\infty. \end{aligned} \quad (3)$$

There is then no physical loss of generality in assuming also that dn/dx is absolutely integrable,

$$dn/dx \in L(\mathbb{R}), \quad (4)$$

which is sufficiently [Olver 1974] to assure solutions of (1) of asymptotic, pure-wave character,

$$v(x) \sim A_{\pm} e^{\pm i\xi/\epsilon} \quad \text{as } \xi = \int_0^x n(s) ds$$

becomes large in magnitude. In turn, this justifies a radiation condition,

$$\begin{aligned} v &\sim e^{i\xi/\epsilon} + r e^{-i\xi/\epsilon} \quad \text{as } \xi \rightarrow -\infty \\ &\sim \tau e^{i\xi/\epsilon} \quad \text{as } \xi \rightarrow \infty \end{aligned}$$

characterizing the desired solution of (1) as an incident wave of unit amplitude plus a reflected wave of amplitude $|r|$ on the far left, and a transmitted wave of amplitude $|\tau|$ on, but no incident wave from, the far right. When this condition is written as

$$\begin{aligned} (v - e^{i\xi/\epsilon}) e^{i\xi/\epsilon} &\rightarrow r \quad \text{as } \xi \rightarrow -\infty \\ v e^{-i\xi/\epsilon} &\rightarrow \tau \quad \text{as } \xi \rightarrow \infty \end{aligned} \quad (5)$$

then (1) to (5) define numbers τ and r , the transmission and reflection coefficients, respectively.

These two complex numbers carry information on both (real) amplitude and phase, and rather different analytical considerations attach to these two aspects. Questions relating to phase will be left aside here to concentrate attention on the amplitudes $|\tau|$ and $|r|$. They are not independent, the natural assumption of real index of refraction implicit in (2), (3) entails an energy-conservation principle for (1) expressed by

$$|\tau|^2 + |r|^2 = 1. \quad (6)$$

The wave problem posed by (1) to (5) is entirely classical and virtually everything is known about its solution [Olver 1974]: it exists, is unique, and if the limits (3) are approached fast enough, can be described to all orders by the WKB approximation

$$n^{1/2} v \sim e^{i\xi/\epsilon} \sum_{n=0}^{\infty} A_n \epsilon^n + e^{-i\xi/\epsilon} \sum_{n=0}^{\infty} B_n \epsilon^n \quad (7)$$

as $\epsilon \rightarrow 0$ for fixed ξ , and by (2), the approximation is even uniform in ξ . This ought to furnish a reliable basis for the calculation of the reflection coefficient, which has been carried out [Chester and Keller 1961] with the following result.

WKB-Corollary 1. If $n(x)$ has k continuous derivatives, except for one finite jump J of $d^k n/dx^k$ at x_0 , and if $d^p n/dx^p$ is absolutely integrable beyond some compact interval for $0 \leq p \leq k+1$, then

$$|r| = [2n(x_0)]^{-k-1} |J| \epsilon^k + o(\epsilon^k).$$

A brief proof is given in the Appendix. The queer aspect of this result is that $|r|$ is determined by the jump of $d^k n/dx^k$, regard-less of any other properties of $n(x)$, which implies a further conclusion [Schelkunoff 1951]:

WKB-Corollary 2. For a smooth index of refraction, with continuous and absolutely integrable derivatives of all orders, there is no reflection, $|r| \sim 0$ to all orders in ϵ .

But, that is puzzling [Mahony 1967] because these theorems place no restriction on the range of $n(x)$, even n_+ and n_- need not be close to each other, and the physical plausibility of partial reflection appears intuitively more related to the range of variation of the index of refraction than to its smoothness? Mathematically, the result is equally paradoxical because a function in the class C^{k-1} can be approximated arbitrarily closely in any plausible norm by a C^∞ -function.

Generations have been tempted to shrug this WKB-Paradox off as, perhaps, merely indicating negligibility of reflection in smooth media. That will not do, however, because inability to calculate reflection implies, by the energy conservation relation (6), that no meaningful information on transmission is at hand either!

Mahony [1967] emphasized, moreover, that the WKB-Corollary 2 implies by no means that $|r|$ is numerically small even when ϵ is so small that successive terms in (7) decrease rapidly with increasing order. A striking example of Olver [1964] illustrating that may, perhaps, be worth quoting at every conference on asymptotics: For large n , the integral

$$I(n) = \int_0^\pi \frac{\cos(nt)}{1+t^2} dt$$

has the (rigorous) asymptotic expansion

$$I(n) \sim (-1)^{n-1} \left(\frac{\lambda_1}{n^2} + \frac{\lambda_2}{n^4} + \frac{\lambda_3}{n^6} + \dots \right)$$

in which all the coefficients λ_i differ little from unity. Since the expansion marches in powers of n^{-2} , successive terms get rapidly smaller and, e.g.,

$$I(10) \sim -0.0005271...$$

with the third and all further terms contributing less than the last digit quoted. Direct computation, however, gives

$$I(10) = -0.0004558... .$$

The error of the expansion therefore exceeds 16% even at $n = 10$, where the expansion had such excellent appearance. Olver [1964] points out that this error is closely accounted for by the term

$$\frac{1}{2} \pi e^{-n}$$

in $I(n)$, which is technically negligible in comparison with all terms in the expansion, but actually exceeds even λ_2/n^4 at $n = 10$.

In the somewhat larger context of this Section, the WKB-paradox provides a healthy comment on a contemporary tendency to consider a problem solved when a close, approximate solution of the pertinent differential equation and boundary conditions has been obtained. For the simple, classical problem just described, we have long known everything about the solution, but almost nothing, about reflection and transmission. The solution $v(x)$, however, cannot usually be observed inside the medium and it has signally failed to point the way towards predicting what can be observed.

II. Central Scattering

One of the earliest and simplest problems of quantum mechanics, which also has classical analogues in many sciences, concerns the motion of a particle in the field of a spherically symmetrical potential $U(r)$. Its stationary states are described [e.g. Landau and Lifshitz 1974] by Schrodinger's equation,

$$\frac{\hbar^2}{2m} \nabla^2 \Psi + [E - U(r)]\Psi = 0$$

for the wave function $\Psi(x,y,z)e^{-iEt/\hbar}$, where m is the mass and E , the energy. It is traditional to split the angular momentum off by the help of spherical harmonics Y_{lm} so that $\Psi = r^{-1}\psi(r)Y_{lm}$ and ψ satisfies a radial Schrodinger equation,

$$\frac{\hbar^2}{2m} \frac{d^2\psi}{dr^2} + [E - U_l(r)]\psi = 0 \quad (8)$$

with 'centrifugally corrected' potential

$$U_l(r) = U(r) + \hbar^2 l(l+1)/(2mr^2) \quad (9)$$

where l is the quantum number of the total angular momentum.

A common type of potential of particular physical and chemical interest is characterized by a central singularity of Coulomb type [Kramers 1926], so that

$$rU(r) \rightarrow -U_0 < 0 \text{ as } r \rightarrow 0, \quad (10)$$

and by a maximum U_m of $U(r)$ at $r = r_m$, say (Fig. 1), whence $U(r)$ falls to a finite value as $r \rightarrow \infty$, which may be chosen as $U = 0$. In physical parlance, this class of potentials is defined by the feature of a central well surrounded by a potential barrier (Fig. 1). It is well known [Landau and Lifshitz 1974] that bound states of energy $E < 0$ may then exist in the well, which are eigenfunctions of (8) for eigenvalues of E and generate resonance in scattering processes. For positive energy, however, the effect of tunneling precludes bound states because the leakage of probability through the barrier implies that any eigenfunction would have to decay in time. Indeed, it is not hard to deduce rigorously from the quantum principle of conservation of total probability for Schrodinger's equation that no real eigenvalue $E > 0$ can exist for a potential of this type [Landau and Lifshitz 1974] and therefore, no resonance can occur at positive energy.

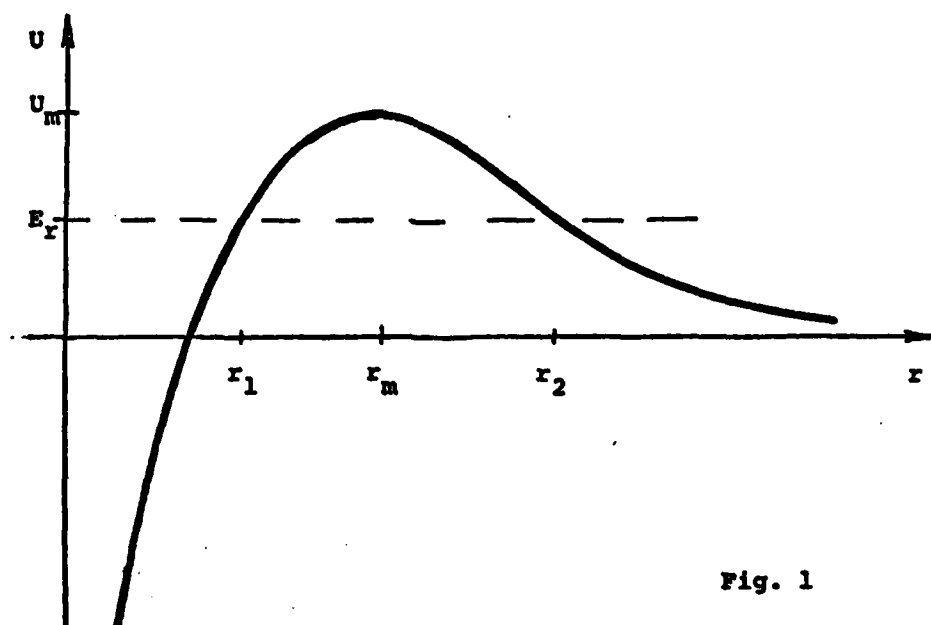


Fig. 1

In the last decades, however, careful scattering experiments have led to the observation of the highest and sharpest resonance spikes precisely for positive energies! The basic explanation of such 'quasiresonant' observations is not difficult: the leakage of probability through the barrier implies radiation damping and therefore, any solutions of Schroedinger's equation in the tunneling range must decay in time. In the notation just sketched, they must therefore have complex values of E , and the characteristic decay time,

$$T = -\hbar / \text{Im} E \quad (11)$$

is called the life of the solution. The tunneling is no one-way street, however, and as outward tunneling leads to radiation damping, so inward tunneling will produce a radiation excitation. The standard measure of such excitation is called response and is defined as follows. The generation of stationary states in the tunneling range requires a supply of radiation from infinity to compensate for the unavoidable radiation damping, and the 'response' is the ratio of the stationary-state amplitude in the well to the supply

amplitude needed to maintain the stationary solution. (Of course, these amplitudes are defined in a mean-square sense because the local amplitude of Ψ varies from point to point.) It is no great surprise to find, when these notions are expressed more quantitatively [e.g. Longuet-Higgins 1967] that the response is directly proportional to the life T . In normal scattering experiments, accordingly, solutions of short life will barely show up, but solutions of long life may be very strongly excited. The key problem for the physicist and chemist is therefore the prediction of the life (11) for those solutions which have a very long life.

Now, this tunneling effect is precisely the mathematical problem for which WKB or turning-point theory was first developed by Kramers [1926], Zwaan [1929] and Langer [1931] and then greatly perfected by many others [Olver 1974, 1978]. It achieved the formidable objective of tracing the solution which is exponentially small in the tunnel reliably through the shadow of the solution which is there exponentially large in the parameter \hbar . The result is an asymptotic expansion of the eigencondition in powers of

$$k^{-2} = \hbar^2 / (2mU_m) , \quad (12)$$

whence an asymptotic expansion

$$E \sim \sum_s e_s k^{-2s} \quad (13)$$

of the eigenvalues can be deduced, and the problem appears solved.

The theory has indeed been successful for inelastic scattering, both in the quantum-mechanical and a classical context [Meyer and Painter 1979], at least as far as the determination of e_0 in (13) is concerned. A closer look at the fine print of the theorems [Evgrafov and Fedoryuk 1966, Olver 1974] reveals technical difficulties [Lozano and Meyer 1976], impeding the determination of e_s for $s > 1$. In any case, however, it has been shown [Lozano and Meyer 1976, Meyer and Lozano 1983] that, for elastic scattering, every coefficient e_s in (13) is real! It follows immediately from (13) and (11) that the theory then yields no information at all on $\text{Im } E$, on the life T , on the response and on the degree of quasisonant excitation.

Of course, if the interpretation of this result turned out to be, in a manner similar to the indications for wave reflection in the preceding Section, that $\text{Im } E$ is 'transcendentally small', $\text{Im } E \sim 0$ to all orders in k^{-2} , then it would be natural that all e_n in (13) are real. It would also mean, however, that the life T and the response to excitation are transcendentally large! The eigenvalues of imaginary part so negligibly small as to fall through even the fine meshes of turning point theory would be precisely the eigenvalues of the greatest interest.

If a brief comment on the lessons of these two examples be permitted, it appears that the WKB-expansions of the respective solutions $v(x)$ and $\psi(r)$ for them may be the correct answer to the wrong question?

The Author's experience, in fact, has been that it is not very rare that asymptotic expansions are of relatively little value outside of mathematics. That is not real heresy, because the basic concept of asymptotics is that of approximation, and if the asymptotic property of a first approximation be proven, then its validity and value depend in no way on approximations of higher order.

From the point of view of mathematical physics, the comment may also be relevant that, more often than not, the solutions of the differential equations are not themselves very observable. This is canonical in quantum mechanics and a closer look at experiment and field observation in a number of sciences indicates that it extends quite far into classical physics. The main observables tend to be quantities of the type of scattering coefficients or resonances, and the two examples indicate that it is not entirely exceptional to find that their prediction requires approximations to both asymptotic quantities of algebraic type (i.e., powers) and of transcendental type (e.g., exponentials).

III. Wave Reflection

The two examples just sketched were among the earlier ones of an increasing number of physical and biological problems encountered in the last decade in which asymptotics of exponential precision was found mandatory. It may therefore be of interest to sketch now the salient points of approaches that proved effective for them. The analysis of wave reflection, in particular, has reached remarkable simplicity and a more general significance of its ideas is indicated by the surprising success with which it has been extended to arbitrarily nonlinear modulation [Meyer 1976a] at the instance of the adiabatic invariance of the magnetic moment in plasma physics.

Of two main steps by which the reflection coefficient $|r|$ of Section I can be obtained, the first consists in no more than the observation that $|r|$ is a number, which must be a functional of the solution $v(x)$ of (1) to (5), and a suitable representation of this functional should be helpful.

The radiation condition (5) indicates that the natural variable for modulation is the Liouville-Green variable

$$\xi/\epsilon = \epsilon^{-1} \int_0^x n(s) ds \quad (14)$$

which measures distance in units of local wave length and is an analog of Hamilton's 'angle'. When the unknown v in (1) is regarded as a function $v(\xi)$, that equation becomes

$$\begin{aligned} d^2 v / d\xi^2 + 2f(\xi) dv / d\xi + \epsilon^{-2} v &= 0, \\ f(\xi) &= \frac{1}{2} n^{-2} dn/dx, \end{aligned} \quad (15)$$

and the reflection coefficient $|r|$ must be a functional of this modulation function f , which is seen to characterize the problem (15), (5) completely.

A representation of that functional has been obtained by many authors in a variety of ways, of which two samples are quoted in [Meyer 1980]. A simple form of it states that the magnitude, even if not the phase, of r is the same as that of

$$a_+ = \int_{-\infty}^{\infty} ([a(\xi)]^2 - 1) e^{-2i\xi/\epsilon} f(\xi) d\xi, \quad (16)$$

where $a(\xi)$ is an auxiliary function defined by the Riccati equation of (1),

$$da/d\xi = \frac{2i}{\epsilon} a + (a^2 - 1)f, \quad a(-\infty) = 0. \quad (17)$$

[The WKB-Corollary 1 of Section I follows (Appendix) from (16), (17) by the stationary phase rules for Fourier transforms without reference to the WKB-representation of v or to details of $a(\xi)$.] As a pointer to the motivation for (16), it may be noted that an integral equation associated in a simple and obvious way with (17) is

$$a(\xi) e^{-2i\xi/\epsilon} = \int_{-\infty}^{\xi} ([a(s)]^2 - 1) e^{-2is/\epsilon} f(s) ds. \quad (18)$$

Like dn/dx , moreover, $f(\xi) \in L(\mathbb{R})$, by (2), (3), (14) and (15), and what questions may attach to the integrals in (16), (18) therefore tend to be not questions of convergence.

Since (17) indicates $a(\xi)$ to be small -- in fact, it is readily proven to be $O(\epsilon)$ -- a common approach to the functional (16) has been to iterate by the help of (17) or (18), starting with $a(\xi) = 0$, so that a first approximation to (16) becomes

$$- \int_{-\infty}^{\infty} e^{-2i\xi/\epsilon} f(\xi) d\xi. \quad (19)$$

That is tricky, however, because the contributions from the oscillatory integrand cancel in this Fourier integral with large parameter $1/\epsilon$ to an extent making the integral smaller than the conjectured error $O(\epsilon^2)$, indeed, smaller than any power of ϵ when $f(\xi)$ is smooth and decays well at ∞ . The other integral in (16),

$$\int_{-\infty}^{\infty} a^2 e^{-2i\xi/\epsilon} f d\xi$$

turns out similarly to be much smaller than $O(\epsilon^2)$, and in the end, a correct execution of this approach yields no more than Corollary 2 of Section I, because the functional (16)

possesses the favorable property of Fourier integrals to such an excessive degree that one is tempted to speak of cancellation sickness.

This diagnosis of the technical root of the WKB-paradox indicates the possibility of an easy cure by the second main step: complex embedding. To this end, it is assumed now that the index of refraction, $n(x)$, is analytic. Lest this appear a drastic restriction, it may be observed that $n(x)$ represents the properties of the medium and must be specified, if not by speculation, then from measurements, which could not support a distinction between analytic and non-analytic functions. A further justification emerges from work on a related functional [Meyer and Guay 1974, Stengle 1977] which indicates the effective approach to non-analytic, smooth functions $n(x)$ to be their approximation by analytic functions.

When $n(x)$ is analytic, the same follows from $f(\xi)$ from (14) and (15), and for $a(\xi)$, from (17) or (18). A rational approach, in fact, is to start from the hypothesis that $f(\xi)$ is analytic on a neighborhood of the real ξ -axis of positive minimum width. This demands an extension of the radiation condition (5) to the analytic strip of $f(\xi)$; a formulation is found in [Meyer 1975] and permits shifting the path of integration in (16) from the real ξ -axis to a parallel path in the lower half-plane. On the new path,

$\text{Im } \xi = \text{const.} = -k$, the offending factor $\exp(-2i\xi/\epsilon)$ in the integrand has very small magnitude $|\exp(-2i\xi/\epsilon)| = \exp(-2k/\epsilon)$, and by pulling this constant factor out of the integral, the cancellations are made explicit.

This cure will be clearly improved by increasing k as far as possible, i.e., by shifting the path down until it encounters the first singularity of $f(\xi)$ (Fig. 2). For simplicity, only one such singular point, $\xi = \xi_c$, will be envisaged here (any finite number of them turn out [Meyer 1975] to make additive contributions to reflection). Figure 2 prompts a conjecture that a principle of stationary phase might apply to the integral (16) on this path, that is, the contributions from the long, straight path segments might be of minor importance. This is the first point where the analysis calls for some work: Simple, contractive estimates on (18) [Meyer 1975] show the conjecture to hold, the major

contribution to reflection arises just from the path indentation at $\xi = \xi_c$ (Fig. 2), if that contribution is of order $\exp(2 \operatorname{Im} \xi_c / \epsilon)$ as $\epsilon \rightarrow 0$, as one would anticipate.

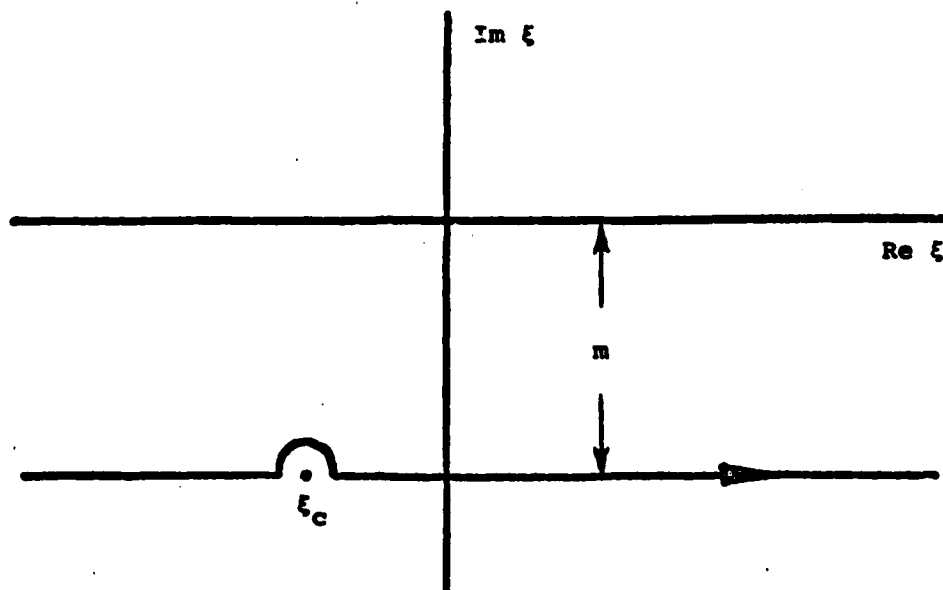


Fig. 2

Observe how the scene has changed, the functional (16) related to reflection is revealed as a local property of the singularity of $f(\xi)$ nearest to the real ξ -axis. (This also explains why knowledge of the WKB-solution (7) of (1) at real x has not been relevant or helpful in the present context.)

The contribution of the indentation to (16) is seen from (18) to be just the jump of $a(\xi)\exp(-2i\xi/\epsilon)$ across ξ_c , so that the remaining piece of the problem is a local WKB-connection. Its solution is needed to confirm the principle of stationary phase for (16), but since the cancellations are already fully explicit, it is needed only to a first approximation. The solution [Langer 1931] has been extended to a very large class of singularities in [Painter and Meyer 1982, Meyer and Painter 1983]. The result of the local computation [Meyer 1975, 1976] is

$$|r| = |a_+| = 2 e^{-2m/\varepsilon} \cos(\mu\pi) + o(e^{-2m/\varepsilon}), \quad (20)$$

where $m = -\text{Im } \xi_c$ (Fig. 2) and the less important parameter μ is related to the branch structure of f at ξ_c . The transmission coefficient $|t|$ is then given by (6).

The main feature of reflection is now seen to be the cancellation factor $\exp(-2m/\varepsilon)$ in (20), in which m/ε may be called the 'wave number characteristic of reflection'. The key parameter $m = |\text{Im } \xi_c|$ is the halfwidth of the analytic strip of $f(\xi)$ and, contrary to intuitive expectations, reflection is now seen not to be closely related to either the range of variation of the index of refraction or to its maximal rate of variation. Though clearly fundamental, the width of the analytic strip is a subtle property of a function. An interpretation [Stengle 1977] that remains applicable well beyond the class of analytic functions is that m characterizes the growth, as $p \rightarrow \infty$, of the L-norm $\|d^p n/dx^p\|$ of high-order derivatives as function of the order p of differentiation.

If the index of refraction $n(x)$ be specified by speculation, m and μ in (20) are, of course, readily read off (14) and (15) [Meyer 1979]. If the index be obtained from measurement, however, the determination of m to a close approximation may pose a problem (and that of μ , may thereby be made moot). That this difficulty is peculiar to very short wavelengths is suggested by a different approach to wave reflection [Gray 1982] which accepts the restriction $c_0 \|f\| < 1$ on the modulation function in order to solve (15),

$$d^2 v/d\xi^2 + \varepsilon^{-2} v = -2f(\xi) dv/d\xi$$

for fixed ε by contraction with the simple, lefthand resolvent. In particular, a power series in $\|f\|$ usually provides an effective algorithm for reflection, as long as the phase velocity $c(x)$ (Section I) varies fairly slowly. The first term in the series for (16) is then indeed (19) and the remainder is smaller by a factor $\|f\|^2$. Under normal circumstances, when the frequency is not all that high and the variation of the index of refraction, not exceptional, reflection therefore appears to be more robust than the shortwave result might suggest.

IV. Quasiresonance

The central scattering problem of Section II is technically harder and has not yet received a treatment of comparable simplicity, but a sketch of the main notions and principles by which it was solved [Lozano and Meyer 1976, Meyer and Lozano 1983] may also be of interest. The discussion of Section II has served mainly to clarify that the important, quasiresonant states are those of long life (11) and that this mandates a search for eigenvalues E of nonzero, but extremely small, imaginary part. So small, indeed, that it could not be pinpointed with any conviction without rigorous proof of their existence.

Since the potential $U(r)$ is real at real radius r , it follows from (9) that the roots of $E - U_l(r)$ must also be slightly complex, and since those are the crucial turning points of the Schrodinger equation (8), it becomes clear that an analysis in two complex variables, E and r is required, in combination with asymptotics in the real parameter \hbar . All experience to-date suggests that it may be a principle of transcendental-precision asymptotics that success depends on avoidance of premature approximation. Once adequate conviction has been attained that a quantity is well-defined, then it can be given a name and the further progress of the analysis need not be impeded by the question of how the quantitative content of this name might be calculated. Indeed, it is likely to become clear only at a quite advanced stage of the analysis which quantities really need to be computed, and to what accuracy. For quasiresonance, in particular, success was first achieved by conducting the analysis in the two complex variables exactly, if somewhat abstractly, and by postponing approximation with respect to \hbar to the very end. This also serves simplicity by avoidance of entanglement with the details and error estimates of approximation.

The first step should clearly be to formulate the eigenvalue problem. The governing equation (8) can be made non-dimensional by measuring energy and potential in units of

$$\max_{r \in \mathbb{R}} U(r) = U_m = U(r_m)$$

(Fig. 1) and distance, in units of r_m . It then becomes

$$\psi'' + k^2(E - U_l)\psi(r) = 0, \quad U_l = U(r) + l(l+1)/(kr)^2, \quad (21)$$

where the large wave number scale k is given by (12),

$$k = (2mU_m)^{1/2} r_m / \hbar .$$

For quasisresonance, attention may now be restricted to angular momenta for which

$2\ell(\ell + 1)/k^2 < \max(r^3 dU/dr)$, so that $U_\ell(r)$ also possesses a well (Fig. 1), to energies in the tunneling range, $0 < \text{Re } E < 1$, and to wave functions satisfying a radiation condition that the wave be purely outgoing at sufficiently large $|r|$.

Next, the potential $U(r)$ needs extension into the complex plane of the radius r , and the reasons mentioned in Section III justify again a restriction to analytic potentials. More precisely, $U(r)$ is assumed analytic on an arbitrarily narrow neighborhood N of $(0, \infty)$, beyond which it may be left undefined. For a clear formulation of the radiation condition, however, N is assumed 'sectorial': for all sufficiently large $|r|$, it is to include an interval of $|\arg r|$ of positive length.

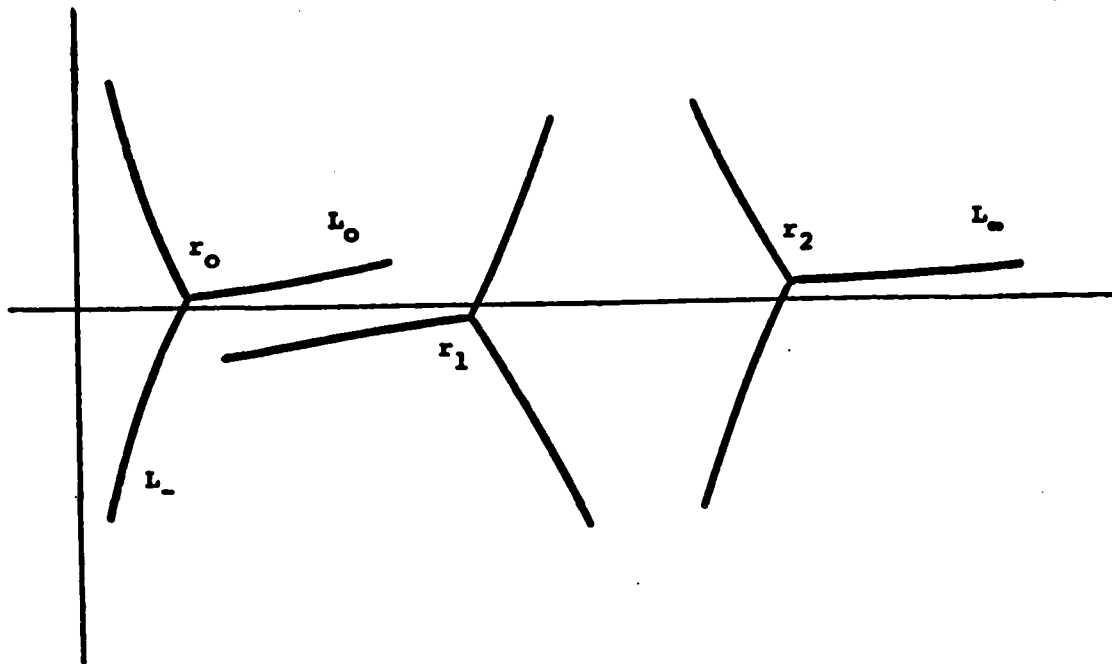


Fig. 3. Turning points and Stokes lines in the complex plane of the radius r .

Figure 3 shows the structure of the r -plane for small $\text{Im } E < 0$ (as it will turn out to be, fortunately, because the analysis has no right to assume its sign). There are three near-real roots r_s of $E - U_l(r)$: two are plain from Fig. 1 and the third, r_0 , lies closer to the origin, where the centrifugal correction $l(l+1)/(kr)^2$ over-powers the Coulomb singularity (10). The figure also shows the Stokes lines L_1 of (21) on which

$$\text{Re} \int_{r_s}^r [E - U_l(t)]^{1/2} dt = 0, \quad s = 0, 1 \text{ or } 2$$

and of which three issue from each of the simple roots r_s (except for $l = 0$, which will be ignored for a while, for brevity). The WKB-theorem [Evgrafov and Fedoryuk 1966, Olver 1974] associates with each Stokes line L_1 a pair of fundamental solutions $u_1(r)$, $v_1(r)$ of (21) which have on L_1 the character of pure progressive waves, undamped and un-amplified with distance from r_s . Let u_1 denote the wave outgoing from r_s along L_1 and v_1 , the incident wave. Both are exact solutions of (21) on all of N , but do not possess the pure wave character on L_j for $j \neq 1$.

The far-field Stokes line L_∞ (Fig. 3) lies close to the real axis and remains in N , which permits a precise formulation of the radiation condition that no incoming wave be present at ∞ : the representation

$$\psi(r) = A_\infty u_\infty(r) + B_\infty v_\infty(r) \quad (22)$$

of the wave function as a linear combination of u_∞, v_∞ must satisfy

$$B_\infty = 0, \quad A_\infty \neq 0. \quad (23)$$

The final condition for elastic scattering is that the wave function Ψ (Section II) must be square-integrable and the same follows for $\psi(r)$. This is effectively a regularity condition at the singular point $r = 0$ (Fig. 1), which will emerge to be interpretable in terms of the 'reflection coefficient'

$$A_0/B_0 = R \quad (24)$$

in the central wave-representation

$$\psi(r) = A_0 u_0(r) + B_0 v_0(r) \quad (25)$$

of the wave function.

Since the fundamental pairs are exact solutions, they must be linearly related, and since (22), (25) represent the same, exact solution $\psi(r)$, it follows that the amplitude coefficients must also be linearly related,

$$\begin{pmatrix} A_\infty \\ B_\infty \end{pmatrix} = S \begin{pmatrix} A_0 \\ B_0 \end{pmatrix}$$

with a 'scattering' matrix $S = ((S_{ij}))$ independent of r . By (23), (24), the exact eigencondition is therefore

$$\begin{aligned} 0 &= B_\infty/B_0 = S_{22} + S_{21} A_0/B_0 \\ &= S_{22} + S_{21} R. \end{aligned} \quad (26)$$

The search for eigenvalues is now seen to involve, not the approximation of the wave function, but the 'connection' question of how fundamental pairs are related.

Schroedinger's equation enters into observable matters only through the three coefficients in (26), and the only concern is how those depend on E and $U(r)$ when k is large, but fixed. The formulation chosen reflects hindsight that this question demands rather different considerations for the singularity at $r = 0$, when the angular momentum l is bounded independently of k , and for the scattering process away from $r = 0$, which is quasiclassical.

The computation of the scattering matrix is precisely the objective of turning-point connection theory, which has established several methods for it, all leading to

$$\begin{aligned} \gamma_0 S_{21} &\sim 1 + \sum_1^{\infty} c_s(E) k^{-s} \\ \gamma_0 S_{22} &\sim \exp[-2k\xi_0] \left\{ 1 + \sum_1^{\infty} d_s(E) k^{-2s} \right\} \end{aligned} \quad (27)$$

as $k \rightarrow \infty$, where $\gamma_0 \neq 0$ is irrelevant to (26) and ξ_0 is a familiar WKB-distance specified in (30) below. A definite algorithm for c_s and d_s has been established only under unrealistic restrictions on the potential [Evgrafov and Fedoryuk 1966], but in any case, (27) only supports (13) and hence, cannot yield any information at all on the life of ψ for elastic scattering. Lozano and Meyer [1976] therefore recalculated S_{21} and

S_{22} more exactly; since Olver's [1978] magnificent 'central-connection' formulation was not yet public at the time of their struggle, they used the 'lateral-connection' approach [Evgrafov and Fedoryuk 1966] in combination with the principle of conservation of probability. This makes $E - U_\ell$ in (21) real when E and r are real, and permits defining some of the wave pairs u_1, v_1 with a complex-conjugate symmetry in the planes of E and r , which is inherited by some of their functionals. $E - U_\ell(r)$ is obviously analytic in E , moreover, and suitable functionals inherit that also. By tracing this analyticity and symmetry painstakingly through the turning-point analysis, Lozano and Meyer [1976] proved the following result.

Precision-Scattering Theorem. For potentials of the type described, the scattering coefficients in (26) can be represented exactly in the form

$$\gamma_0 S_{21} = i \exp[i\mathcal{E}_1(E, k)/k] - (1 + i)\{1 + \Omega(E, k)/k\} e^{-2k\xi_1}, \quad (28)$$

$$\gamma_0 S_{22} = e^{-2k\xi_0} \exp[i\mathcal{E}_2(E, k)/k], \quad (29)$$

with

$$\mathcal{E}_0(E, k) = \int_{r_0}^{r_1} [F_0(r)]^{1/2} dr, \quad (30)$$

$$F = U_\ell(r) - E$$

$$\mathcal{E}_1(E, k) = -\int_{r_1}^{r_2} [F_1(r)]^{1/2} dr, \quad (31)$$

(where the subscripts on F denote an appropriate determination of branches of the root) and with $\gamma_0 \neq 0$, $\mathcal{E}_j(E, k)$ analytic in E and real for real E , and \mathcal{E}_j and $\Omega(E, k)$ bounded as $k \rightarrow \infty$.

The crucial, new feature is here the term in (28) with factor $\exp(-2k\xi_1)$, which is exponentially small because ξ_1 turns out to be real positive when E is real. Such a term would be meaningless in (27), but the additional information on \mathcal{E}_1 shows the first

term in $\gamma_0 S_{21}$ to be of exactly unit magnitude. The very small term therefore describes at real E the difference between $|\gamma_0 S_{21}|$ and unity, regardless of the much larger uncertainty about $\arg(\gamma_0 S_{21})$. It is precisely this exponentially small term in (28) which will emerge as the source of all the information on the life T , and this illuminates how the standard, technical meaning of larger and smaller in asymptotics can be misleading.

So, it is the principle of conservation of probability which generates the symmetry on which exponential precision in shortwave scattering can be founded. (In classical scattering [Lozano and Meyer 1976], conservation of energy plays an analogous role.)

For short waves, the most prominent quantities in the Theorem are the WKB-integrals (30), (31). An appropriate determination of branches of $p^{1/2}$ has been worked out by Lozano and Meyer [1976] and shows $k\xi_0 \exp(-i\pi/2)$ and $k\xi_1$ to be real positive at real energy E . The former may therefore be interpreted as the width of the potential well of $U_\ell(r)$ in (21) at the level E in units of local, radial wavelength. Were not the potential barrier just the place where there are no waves, $k\xi_1$ would be similarly interpretable as the potential-barrier width of U_ℓ in such units.

This leaves the reflection coefficient R in the eigencondition (26) to be analyzed, and Meyer and Lozano [1983] have treated the case where the angular momentum ℓ is 'small', i.e., bounded independently of the wave number scale k , and the case where ℓ is so large that $\ell/k \rightarrow \text{limit} > 0$ as $k \rightarrow \infty$. The latter case is quasiclassical, the third turning point, r_0 , is a simple one, near which the solution of (21) is close to an Airy function, the condition of square integrability picks out the correct Airy function, and the well-known solution [Kramers 1926, Olver 1974] of the WKB-connection problem for such a simple turning point yields

$$R = e^{-i\pi/2} + O(k^{-1}) .$$

Unfortunately, this result is again inadequate for information on the life T because its degree of accuracy destroys the chance of using the new information of the Precision Scattering Theorem meaningfully in the eigencondition (26). Nor would further terms in the asymptotic expansion of R help in that respect. But, Lozano and Meyer [1976] pointed out that the principle of conservation of probability for (21) permits normalization of the

fundamental pair u_0, v_0 in (25) so that

$$v_0(\bar{r}) = \overline{u_0(r)}$$

at real E , and since it also makes the wave function ψ real at real E and r , all the unknown error terms must be arrangeable in complex-conjugate pairs, whence they deduce that $|R| = 1$ exactly at real energy. The analyticity in E then implies an exact representation

$$R = e^{-i\pi/2} \exp[ik^{-1} \Sigma_0(E, k)] \quad (32)$$

with Σ_0 again analytic in E , bounded as $k \rightarrow \infty$, and real for real E .

The case of small angular momentum is more complicated because r_0 then moves to within $O(k^{-2})$ of the central, singular point $r = 0$ of (21), and that singularity now over-shadows the embryonic turning-point structure at r_0 . Fortunately, a great deal is known about this Coulomb-singularity [Kramers 1926, Olver 1974] and the connection results for it have been extended to a large class of other singularities by Painter and Meyer [1982] and Meyer and Painter [1983]. For sufficiently small $|r|$, the solutions of (21) are close to Bessel functions, of which the square-integrability condition picks the correct one, and a sufficiently careful comparison with (25) [Kramers 1976, Meyer and Lozano 1983] yields

$$R = e^{-i\pi(1/2 + 2\sigma)} + O(k^{-1/2})$$

with

$$\sigma(l) = l + \frac{1}{2} - [l(l+1)]^{1/2}. \quad (33)$$

This is again inadequate for information on the life, but the same probability-conservation argument as for the case of large angular momentum shows that there must be an exact representation

$$R = e^{-i\pi(1/2 + 2\sigma)} \exp[ik^{-1/2} \Sigma_0(E, k)] \quad (34)$$

with another function Σ_0 of the same properties as in (32).

This result extends to $l = 0$, if the assumption [Landau and Lifshitz 1974] $\psi(0) = 0$ is added for that case, and the angular-momentum correction (33) to the phase shift of central reflection is then massive. For $l > 1$, however, it is quite small and decreases with increasing l , and (34) recovers (32) when $l = O(k)$.

One cannot help feeling that all these technicalities are more complicated than they ought to be and, while hard analysis is surely unavoidable, somebody might be able to straighten it out drastically by the help of just the right integral equation for (21)? In any case, the results at hand are sufficient for an exponentially precise evaluation of the eigencondition. When (28), (29) and (34) are substituted in (26), it is natural to split the characteristic form of (26),

$$\Delta(E, k) = S_{22} + S_{21} R ,$$

into a term collecting all the functions whence asymptotic contributions of algebraic type in k^{-1} are to be anticipated and another term that is exponentially small in k :

$$\Delta(E, k) = i\gamma_0^{-1} R \{ \Delta_0(E, k) + \Delta_1(E, k) \} , \quad (35)$$

$$\Delta_0 = \exp[-2k\xi_0 + 2\pi i\sigma + iE_2/k - iE_0/k^{1/2}] + \exp(iE_1/k) , \quad (36)$$

$$\Delta_1 = (1 - i)(1 + \Omega/k)\exp(-2k\xi_1) . \quad (37)$$

To establish now those elusive eigenvalues E responsible for quasisonance, it is convenient to begin with the real roots E_r of Δ_0 . Since the appropriate branch in (30) makes $\xi_0(E, k) = i|\xi_0|$ for real E , it follows straightaway from (36) that those roots are given by

$$k|\xi_0(E_r, k)| + (E_1 - E_2 + k^{1/2}E_0)/(2k) = (n + \frac{1}{2} + \sigma)\pi \quad (38)$$

which is just the nondimensional form of the quasiclassical quantization rule ignoring the radiation damping [Kramers 1926, Keller 1958], with Kramers' [1926] angular-momentum correction σ . The new feature that it is an exact version of the quantization rule is not of much direct help, because no practical algorithm for the evaluation of the E_1 has been worked out. The feature of immediate relevance is that, since $U(r)$ is monotone increasing on $(0, r_m)$ (Fig. 1), this quantization rule is known to determine a unique, real $E_r(n)$ for large k and given integer n such that still $E_r(n) < U_m$.

The analyticity in E now permits application of the principle of the argument [Lozano and Meyer 1976] to prove existence of a unique, simple root E_n of Δ close to $E_r(n)$ for all sufficiently large k and n . It then follows immediately that, to a first approximation as $k \rightarrow \infty$,

$$\begin{aligned}
E_n - E_r(n) &\sim -\Delta_1(E_r, k) / \Delta_0'(E_r, k) \\
&\sim -\frac{1}{2} (1 + i) [k |\xi_0'(E_r, k)|]^{-1} \exp[-2k\xi_1(E_r, k)]
\end{aligned}
\quad (39)$$

where

$$\xi_0'(E_r, k) = \frac{1}{2} e^{i\pi/2} \int_{r_0}^{r_1} |E_r - U_k(r)|^{-1/2} dr \neq 0. \quad (40)$$

The real part of (39) has little direct meaning, but the imaginary part gives the first approximation to the life (11). In the original, dimensional notation of Section II, it is

$$T_n \sim (8m/U_m)^{1/2} |\xi_0'(E_r(n), k)| \exp[(8mU_m)^{1/2} \xi_1(E_r(n), k) / \hbar] \quad (41)$$

which confirms the conjecture (Section II) that elastic scattering generates eigenfunctions of a life exponentially large in \hbar . It also shows that the computation of such lives requires no more than evaluation of the two definite integrals (31), (40) of typical WKB-type, once the real part, $E_r(n)$, of the eigenvalue E_n has been determined from the quantization rule.

V. Reforms?

The objective of Sections I and II was to explain scientific reasons for attention to some modern questions attaching to old and elementary, linear mathematics. One problem, at least, of fully non-linear oscillator modulation [Meyer 1976a] has greatly reinforced those reasons. Now that initial answers to such high-precision questions have been sketched in Sections III and IV, one wonders about lessons of more general significance that might be drawn from them beyond those noted in the preceding Sections, namely relative unimportance of asymptotic expansion, but importance of complex embedding and of postponement of approximation.

One indication that has impressed the Author is that the conventional comparison between those asymptotic contributions which are algebraically small and those, which are transcendently small, can miss the point. Quasiresonance furnishes a particularly good example, for the answer to one of its two key questions, viz. the eigenfrequency, depends entirely on asymptotics of algebraic type, while that to the other key question, viz. the resonant excitation, depends entirely on asymptotics of exponential type. There are occasions, then, on which a more fruitful view of the distinction between 'algebraically small' and 'transcendently small' may be that this distinction is qualitative more than quantitative.

A second experience which has impressed the Author is that the real observables, in both examples, can be identified with local properties of singular points of the differential equations. (In quasiresonance, most of the points in question are turning points, but the conventional distinction between those and singularities is all too superficial, in any case; it disappears in any intrinsic formulation, such as (15).) It would appear natural to see a more general significance in that experience, once a complex domain for the equations is envisaged.

In regard to wave modulation and scattering, it would also appear significant that the real concern of all the hard analysis, in both examples, was not with the approximation of the solutions of the differential equations, but with the connection of wave amplitudes across the singular points of primary relevance to the problem. It cannot fail to obtrude

during the technical work, as will surely have become clear between the lines of Section IV, that the present form of connection theory is laborious, largely because it involves so much detail. The final results, on the other hand, do not really substantiate the need for all the detail, which has greatly discouraged acquaintance with this branch of asymptotics and thereby made it the preserve of a rather small circle of specialists. Does it deserve the discredit or could it be reformed to the wider benefit of asymptotics?

Turning-point theory is also not very general, even the great monograph [Olver 1974] treats only the simplest types of transition points. Physics motivates such a restriction in the example of quasisonance, but not, in that of wave reflection. The index of refraction of a medium is not ours to choose, but ours to accept as we find it. Since its singular points dominating reflection lie well off the real axis of distance, physics places scant restrictions on their structure. There is no good reason why they should belong even to the class of 'fractional transition points' [Langer 1931, Olver 1977]. Accordingly, the mathematical principle of generalization might here be helpful by mandating abandonment of detail and thereby promoting simplicity and a chance for guidance towards the nucleus of connection and scattering. Such an attempt has been prompted by the work sketched in Sections III, IV, and it may be worth closing this article with a brief sketch of the results and experiences to which it has led.

On present evidence, the overriding lesson seems to be that wave-amplitude connection may be characterized as an asymptotic expression of the branch structure of the singular point [Olver 1974, Meyer and Painter 1983].

To carry this lesson from regular points of differential equations [Olver 1974] beyond the realm where detail is accessible, Meyer and Painter [1983a] studied the branch structure of almost the whole class of irregular points of linear, physical wave- or oscillator-modulation equations. In contrast to all the earlier work on isolated singular points, the new study focuses on 'very irregular' points which are branch points of arbitrary structure. The large class of equations admitted is such that each singular point can be linked by a diffeomorphism to a regular point of the same differential

equation. This led them to 'irregularity bounds' on the quantitative degree of homotopic deformation of regular solution structure as the diffeomorphism is traced to an irregular point.

An incidental discovery (for them, if not perhaps for every Reader) was that the independent variable in (1) or (20) plays two quite different roles in the local solution structure near the singular point. More precisely, this applies to the natural variable ξ in (14), which plays the role of a modulation variable, while ξ/ϵ plays the role of an oscillation variable. Of course, this recalls immediately the notion of slow time and fast time in multiscale asymptotics. The surprise was the discovery of it in an analysis having nothing to do with asymptotics: Meyer and Painter [1983a] study the 'parameter-less' case of the theory of differential equations, in which $\epsilon = 1$, without loss of generality. The two variables, moreover, played completely different roles, not in the asymptotic solution structure (which their investigation left undefined), but in the local structure at the singular point. It would appear that the multiscale notion is anchored much more deeply in the singularity-structure of a class of differential equations than had been realized widely.

The reason for this foray into pure mathematics was the conjecture that, even in the more general context, connection is an asymptotic expression of local branch structure. Accordingly, an adequate representation of local structure should suffice for asymptotic connection of wave amplitudes, and some of the central concepts of present turning-point theory might be irrelevant to that purpose? Indeed, the new theory gives up both the ideas of comparison equation and of uniform approximation. The reason is that the class of fractional transition points stands in one-one correspondence [Langer 1931] to the class of Bessel functions. Once more general singular points are admitted, uniform approximations of similar usefulness cannot exist. That is a pity, for sure, but is unavoidable and eliminates temptation of detail. The comparison equation loses its usefulness similarly. Instead, there is the new idea of a diffeomorphism from regular to irregular points of the same differential equation.

But, how is asymptotic connection to be deduced from knowledge of no more than local structure at the singular point? Meyer and Painter [1983] show that the two-variable structure can provide the key. They use the 'irregularity bounds' on the extent of departure of irregular-point structure from regular-point structure to prove that the two-variable nature of the solutions assures distances from the singular point at which local structure has not yet been lost, but asymptotic structure is already present. In effect, a typical boundary-layer concept has surfaced suddenly: those bounds document 'overlap' between the domains of local and asymptotic approximation, and it is no great surprise that the asymptotic connection formulae then follow immediately from the local branch structure.

Appendix

For a brief proof of Chester and Keller's [1961] WKB-Corollary 1 (Section I), it is again best to ignore the WKB-representation of the solution $v(x)$ of (1) and to start from (16), of which a brief proof is found, e.g., in [Meyer 1975]. From (14) and (15),

$$d^p f / d\xi^p = \frac{1}{2} n^{-p-2} d^{p+1} n / dx^{p+1} + \dots,$$

where dots denote terms involving only derivatives of lower order than those displayed, so that

$$[d^{k-1} f / d\xi^{k-1}] = \frac{1}{2} (n(x_0))^{-k-1} J$$

where $[\phi]$ denotes the jump of ϕ at x_0 , $[\phi] = \phi(x_0 + 0) - \phi(x_0 - 0)$. Since

$f(\xi) \in L(\mathbb{R})$, it follows from (17) or (18) that $a(\xi)$ exists [e.g., Coddington and Levinson 1955], is bounded, in fact, is $O(\epsilon)$, and has one more continuous derivative than $f(\xi)$ does. If

$$\begin{aligned} (a^2 - 1)f &= \Lambda(\xi; \epsilon), \\ d^p \Lambda / d\xi^p &= (a^2 - 1) d^p f / d\xi^p + \dots + 2af d^p a / d\xi^p \\ &= (a^2 - 1) d^p f / d\xi^p + \dots + 2af d^{p-1} (2ia/\epsilon + \Lambda) / d\xi^p \end{aligned}$$

by (17), so that

$$[d^{k-1} \Lambda / d\xi^{k-1}] = -\frac{1}{2} n^{-k-1} J \{1 + O(\epsilon^2)\}$$

and $d^p \Lambda / d\xi^p$ is continuous for $p \leq k-2$ and also, for $p = k-1$ except at x_0 , and has absolutely integrable skirts for $p \leq k$. These properties support the stationary-phase evaluation [Jones 1966] as $\epsilon \rightarrow 0$ of

$$a_+ = \int_{-\infty}^{\infty} \Lambda(\xi; \epsilon) e^{-2i\xi/\epsilon} d\xi$$

to the extent of

$$a_+ = (-i\epsilon/2)^k [d^{k-1} \Lambda / d\xi^{k-1}] + o(\epsilon^k),$$

and $|r| = |a_+|$.

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